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Title: LANL Spectroscopic Modeling of Outputs

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LANL Spectroscopic Modeling of Outputs

Los Alamos is working on the further development of existing capabilities initially built for X-ray spectroscopy (postprocessing ***RAGE*** *for the DIME project) and extending them to the infrared, visible, and ultraviolet regimes.*

To this end, LANL is expanding its area of expertise beyond atomic physics into molecular physics and opacities.

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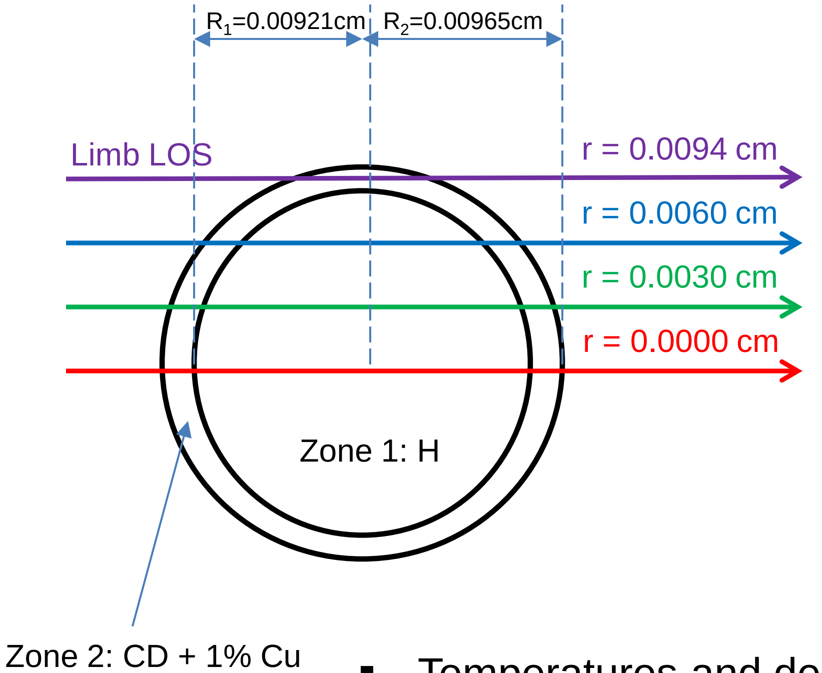
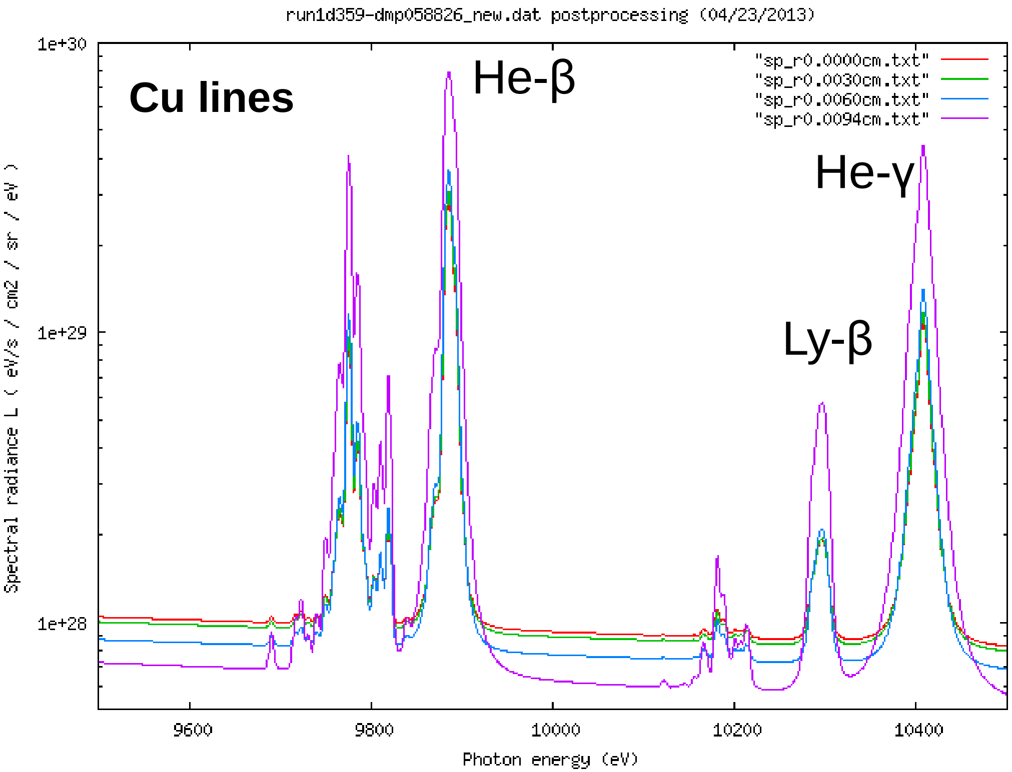
Starting point: postprocessing ICF simulations

FESTR model and code (currently 1-D, steady-state):
Finite-**E**lement **S**pectroscopic **T**ransport of **R**adiation



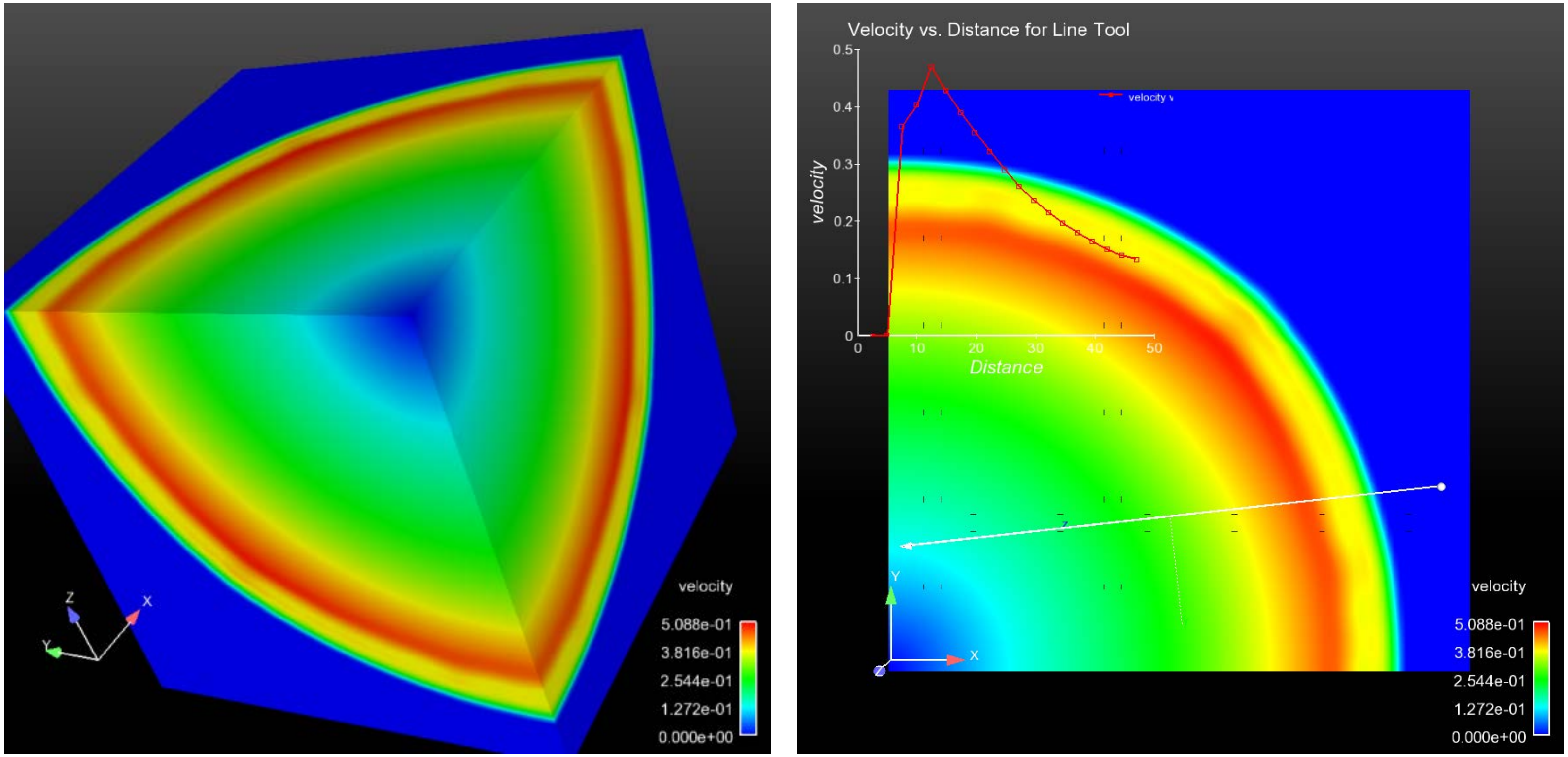


- Temperatures and densities (from RAGE) in each spatial zone are used by the ATOMIC[1] code to calculate mixed emissivities and opacities.
- The radiation transport equation is then solved to generate spectra.[2,3]

[1] M.E. Sherrill et al., Physical Review E **76**, 056401 (2007).
[2] P. Hakel et al., Physics of Plasmas **21**, 063306 (2014).
[3] J.A. Baumgaertel et al., Physics of Plasmas **21**, 052706 (2014).

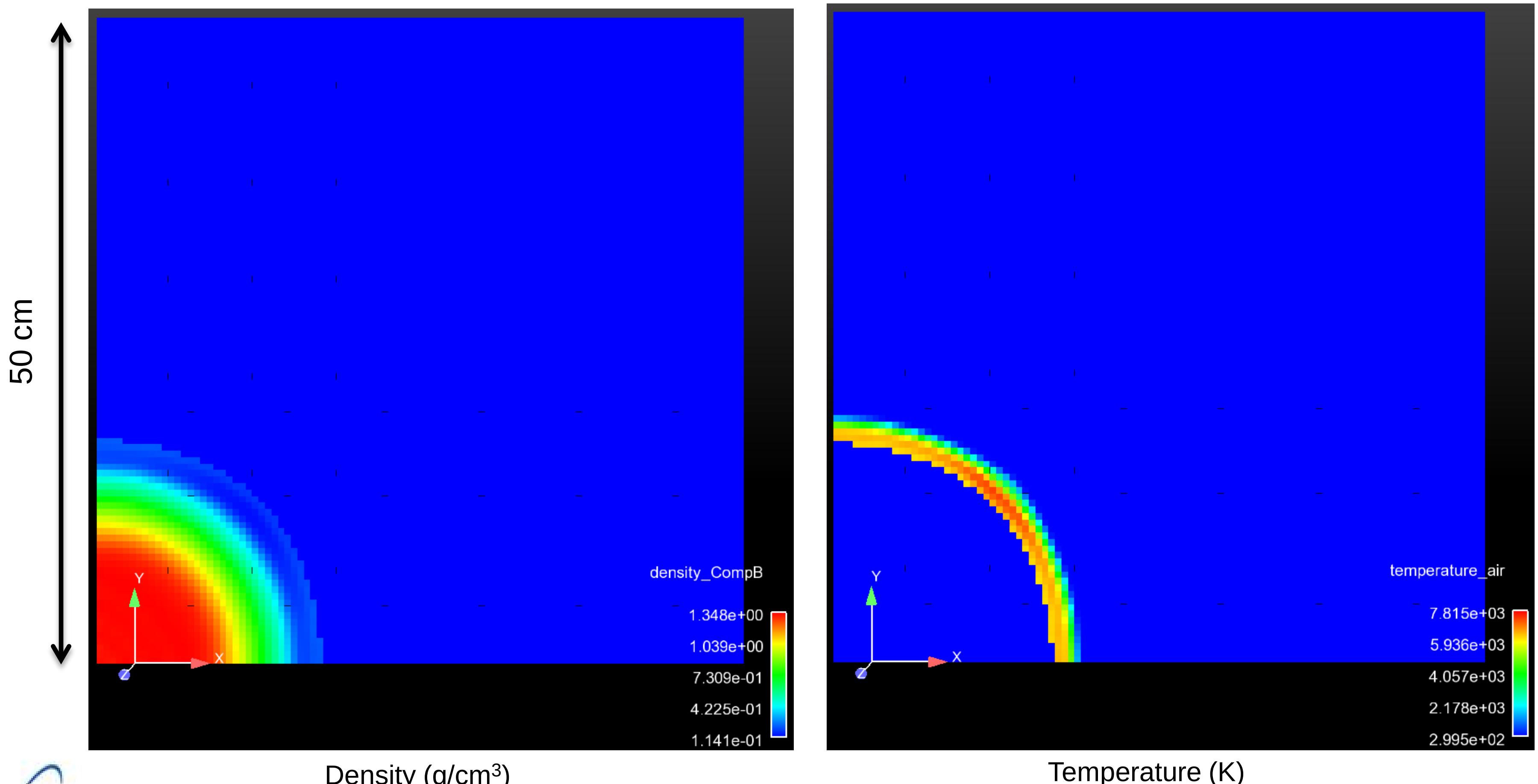
Spectral postprocessing of Pagosa simulations

- Relevant quantities (temperatures, densities, etc.) can be extracted from Pagosa dumps with EnSight visualization software, and saved into files.
- These files then can serve as input for spectral post-processing calculations.



Pagosa results were provided by Jim Reynolds.

Example of a Pagosa run modeling CompB



Pagosa results were provided by Jim Reynolds.

Prototype model as input for FESTR

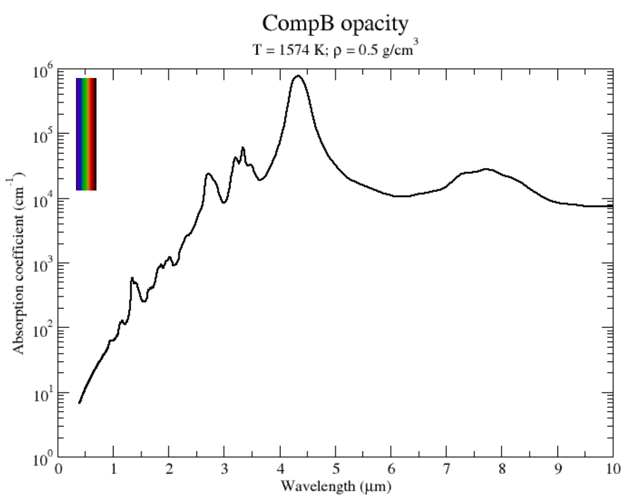
CompB:
T = 1574 K
ρ = 0.5 g/cm^3
thin shell, radius 15 cm
spherical geometry

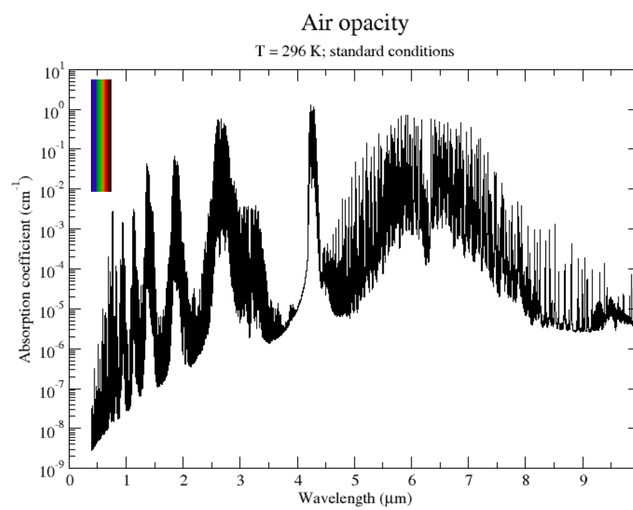
Air:
T = 296 K
standard conditions
length 100 m
planar geometry

Source (“fireball”)

Transport medium (air)

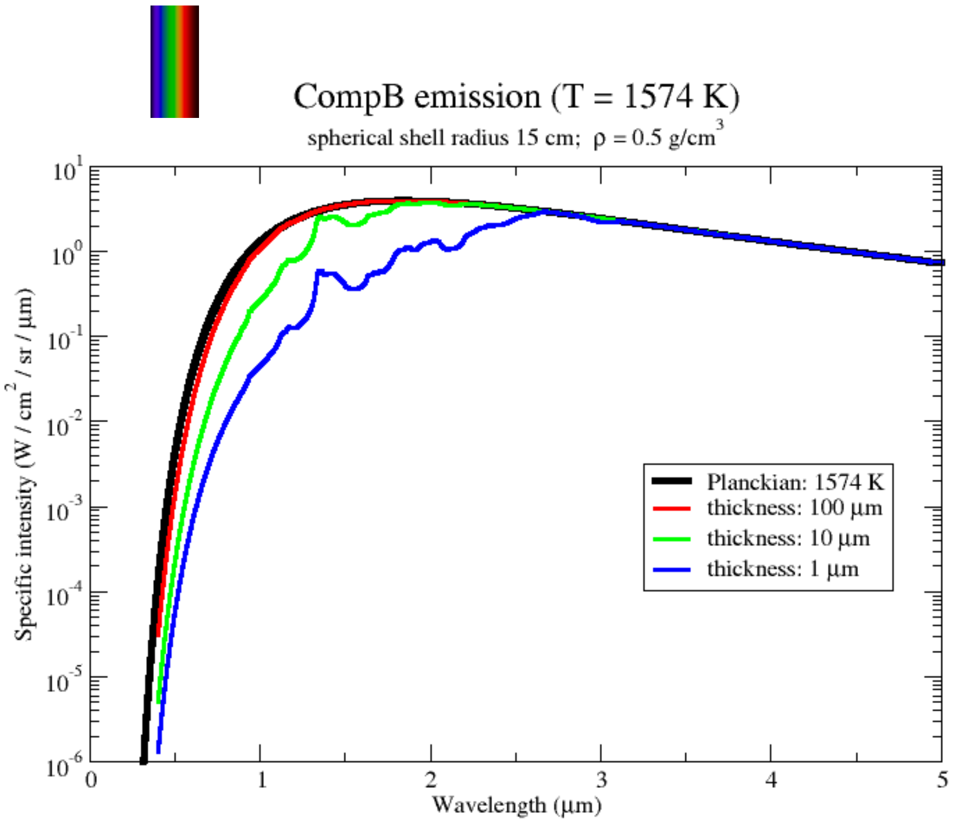
Synthetic spectrum (“detector”)





Opacity data were provided by Eddy Timmermans with Josh Coe, Dima Mozyrsky, Leanne Duffy, and Cristiano Nisoli using the HITRAN molecular database.

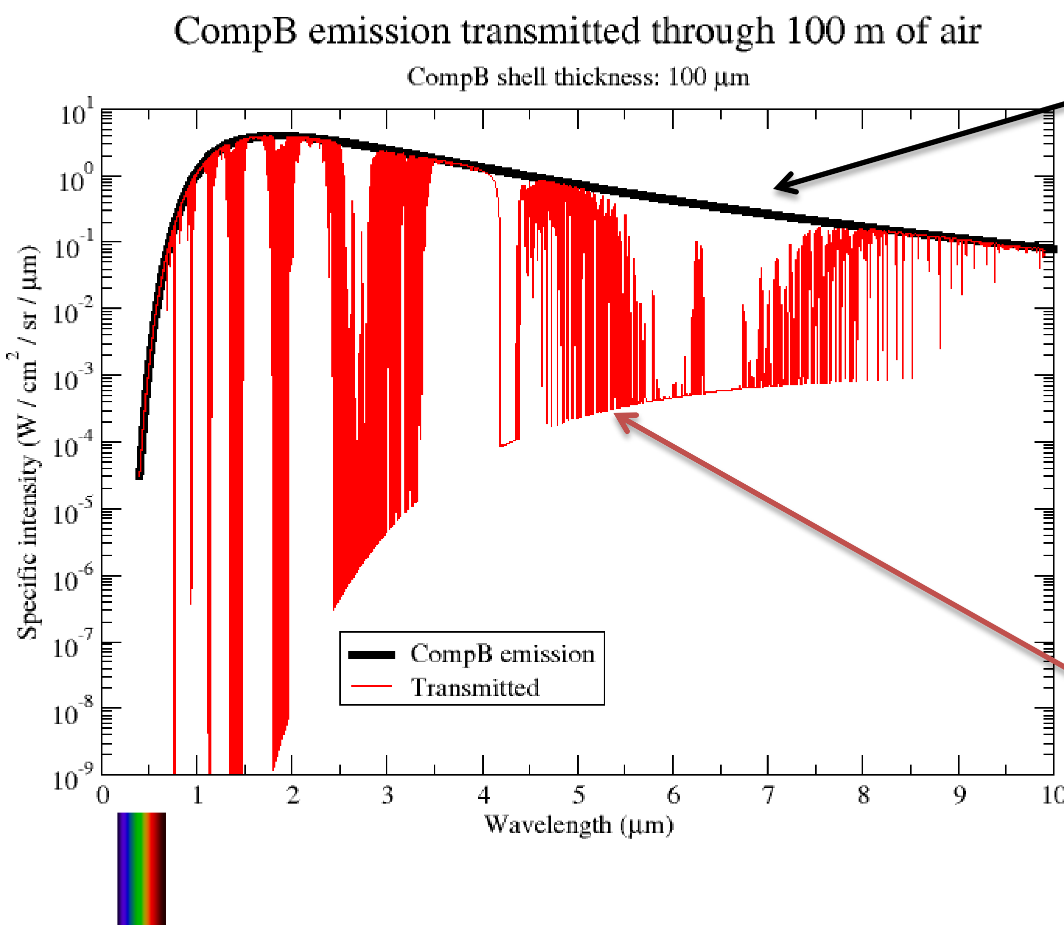
CompB self emission: three shell thicknesses



High opacity

Blackbody spectrum:
i.e., the identity of the material (encoded in its spectral characteristics) can be obscured by the thermalization of the output signal.

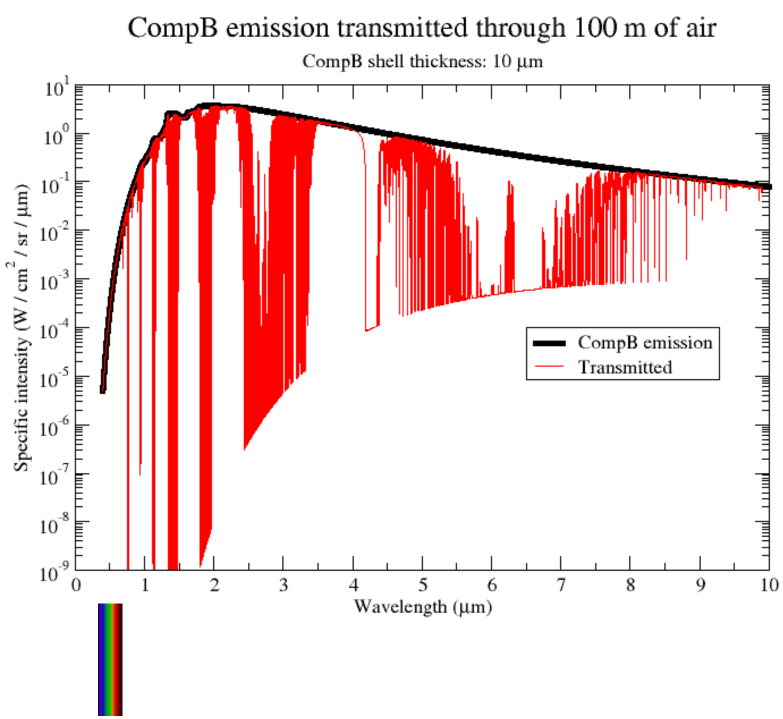
Transmission through air

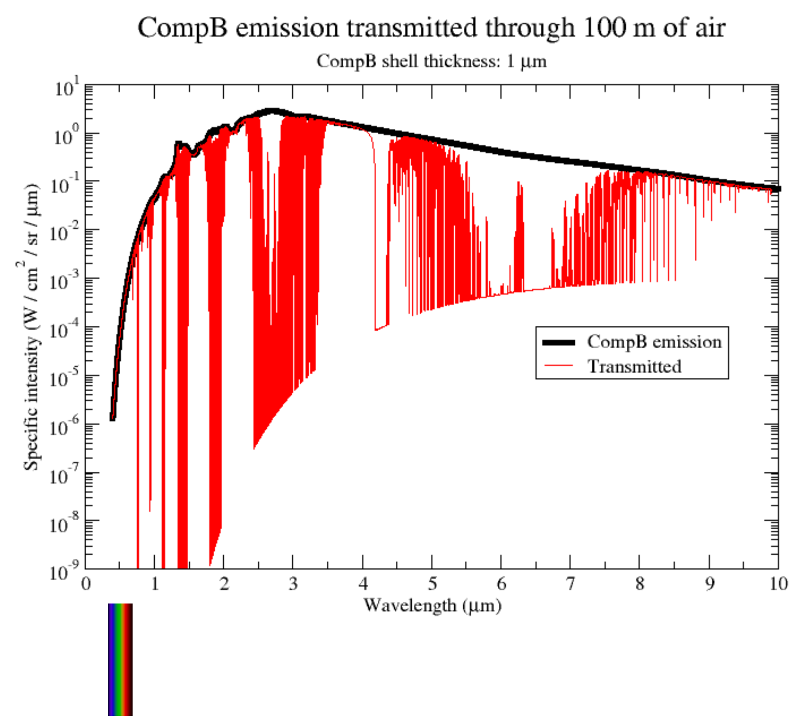


Spectrum no higher than the T = 1574 K Planckian (CompB)

Spectrum no lower than the T = 296 K Planckian (air)

Transmission through air





Summary

- A prototype model and code (FESTR) to calculate spectroscopic-quality outputs exists.
- FESTR currently handles 1-D and steady-state modeling; work is under way to generalize it.
- An effort to supply FESTR with opacities for molecular materials and their mixtures is ongoing.
- Hydrodynamic simulations (e.g., with Pagosa, RAGE, …) can be performed to calculate the state of the relevant materials during output generation.
- Opacities need to access those regions of the parameter space suggested by the hydrodynamic simulations.